```
* * * * * * * * * *   Welcome to STN International   * * * * * * * * * *

 NEWS  1            Web Page URLs for STN Seminar Schedule - N. America
 NEWS  2            "Ask CAS" for self-help around the clock
 NEWS  3   May 12   EXTEND option available in structure searching
 NEWS  4   May 12   Polymer links for the POLYLINK command completed in REGISTRY
 NEWS  5   May 27   New UPM (Update Code Maximum) field for more efficient patent
                    SDIs in CAplus
 NEWS  6   May 27   CAplus super roles and document types searchable in REGISTRY
 NEWS  7   Jun 22   STN Patent Forums to be held July 19-22, 2004
 NEWS  8   Jun 28   Additional enzyme-catalyzed reactions added to CASREACT
 NEWS  9   Jun 28   ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG,
                    and WATER from CSA now available on STN(R)

 NEWS EXPRESS   MARCH 31 CURRENT WINDOWS VERSION IS V7.00A, CURRENT
                MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),
                AND CURRENT DISCOVER FILE IS DATED 26 APRIL 2004
 NEWS HOURS     STN Operating Hours Plus Help Desk Availability
 NEWS INTER     General Internet Information
 NEWS LOGIN     Welcome Banner and News Items
 NEWS PHONE     Direct Dial and Telecommunication Network Access to STN
 NEWS WWW       CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

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  * * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 15:26:37 ON 09 JUL 2004

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                     0.21       0.21

FILE 'REGISTRY' ENTERED AT 15:26:43 ON 09 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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Property values tagged with IC are from the ZIC/VINITI data file
provided by InfoChem.

STRUCTURE FILE UPDATES:     8 JUL 2004  HIGHEST RN 706430-72-0
DICTIONARY FILE UPDATES:    8 JUL 2004  HIGHEST RN 706430-72-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
```
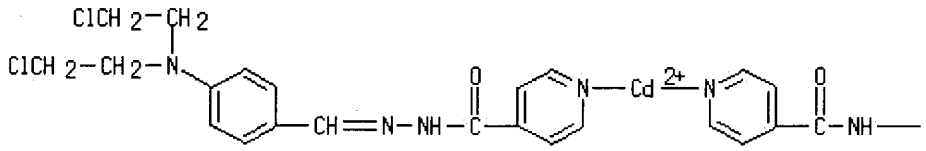

conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

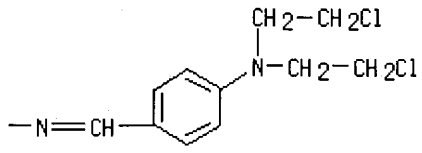
Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

```
=> e  310427-67-9/rn
E1            1     310427-65-7/RN
E2            1     310427-66-8/RN
E3            1 --> 310427-67-9/RN
E4            1     310427-68-0/RN
E5            1     310427-69-1/RN
E6            1     310427-70-4/RN
E7            1     310427-71-5/RN
E8            1     310427-72-6/RN
E9            1     310427-73-7/RN
E10           1     310427-74-8/RN
E11           1     310427-75-9/RN
E12           1     310427-76-0/RN

=> s e3
L1            1 310427-67-9/RN

=> d l1

L1   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   310427-67-9  REGISTRY
CN   Cadmium(2+), bis[(4-pyridinecarboxylic acid-κN1)
     [[4-[bis(2-chloroethyl)amino]phenyl]methylene]hydrazide]- (9CI)  (CA INDEX
     NAME)
MF   C34 H36 Cd Cl4 N8 O2
CI   CCS, COM
SR   CA
```

PAGE 1-A



PAGE 1-B



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E3            1 --> 310427-65-7/RN
E4            1     310427-66-8/RN
E5            1     310427-67-9/RN
```

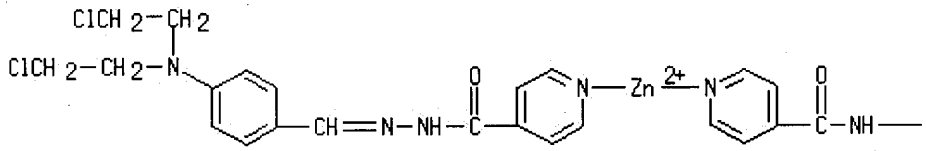
```
E6            1      310427-68-0/RN
E7            1      310427-69-1/RN
E8            1      310427-70-4/RN
E9            1      310427-71-5/RN
E10           1      310427-72-6/RN
E11           1      310427-73-7/RN
E12           1      310427-74-8/RN

=> s e3
L2            1 310427-65-7/RN

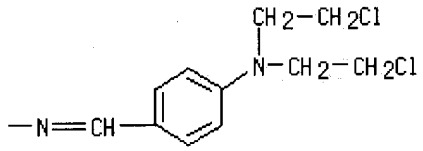
=> d l2

L2   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   310427-65-7  REGISTRY
CN   Zinc(2+), bis[(4-pyridinecarboxylic acid-κN1) [[4-[bis(2-
     chloroethyl)amino]phenyl]methylene]hydrazide]- (9CI)  (CA INDEX NAME)
MF   C34 H36 Cl4 N8 O2 Zn
CI   CCS, COM
SR   CA
```

PAGE 1-A



PAGE 1-B



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E3            1 --> 10325-94-7/RN
E4            1      103250-00-6/RN
E5            1      103250-01-7/RN
E6            1      103250-02-8/RN
E7            1      103250-03-9/RN
E8            1      103250-04-0/RN
E9            1      103250-05-1/RN
E10           1      103250-06-2/RN
E11           1      103250-07-3/RN
E12           1      103250-08-4/RN

=> s e3
L3            1 10325-94-7/RN

=> d l3

L3   ANSWER 1 OF 1  REGISTRY  COPYRIGHT 2004 ACS on STN
RN   10325-94-7  REGISTRY
CN   Nitric acid, cadmium salt (8CI, 9CI)  (CA INDEX NAME)
```

```
OTHER CA INDEX NAMES:
CN   Cadmium nitrate (7CI)
OTHER NAMES:
CN   Cadmium dinitrate
CN   Cadmium nitrate (Cd(NO3)2)
CN   Cadmium(II) nitrate
DR   14177-24-3
MF   Cd . 2 H N O3
CI   COM
LC   STN Files:   AGRICOLA, ANABSTR, AQUIRE, BIOBUSINESS, BIOSIS, BIOTECHNO,
       CA, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMCATS, CHEMLIST, CIN, CSCHEM,
       CSNB, DETHERM*, EMBASE, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE,
       MRCK*, MSDS-OHS, NIOSHTIC, PDLCOM*, PIRA, PROMT, RTECS*, TOXCENTER,
       USPAT2, USPATFULL
         (*File contains numerically searchable property data)
     Other Sources:   DSL**, EINECS**, TSCA**
         (**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA  CAplus document type:  Conference; Dissertation; Journal; Patent; Report
RL.P   Roles from patents:  ANST (Analytical study); BIOL (Biological study);
       MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC
       (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses);
       NORL (No role in record)
RLD.P  Roles for non-specific derivatives from patents:  PROC (Process); RACT
       (Reactant or reagent); USES (Uses)
RL.NP  Roles from non-patents:  ANST (Analytical study); BIOL (Biological
       study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU
       (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT
       (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents:  BIOL (Biological
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       reagent); USES (Uses)
CRN  (7697-37-2)
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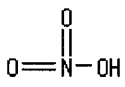

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 # 1/2  Cd
            1477 REFERENCES IN FILE CA (1907 TO DATE)
              19 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
            1480 REFERENCES IN FILE CAPLUS (1907 TO DATE)
               1 REFERENCES IN FILE CAOLD (PRIOR TO 1967)


=>
 * * * * * * RECONNECTED TO STN INTERNATIONAL * * * * * *
SESSION RESUMED IN FILE 'REGISTRY' AT 15:39:18 ON 09 JUL 2004
FILE 'REGISTRY' ENTERED AT 15:39:18 ON 09 JUL 2004
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COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                14.13      14.34

=> file casreact
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                                14.97      15.18
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FILE 'CASREACT' ENTERED AT 15:40:30 ON 09 JUL 2004
USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

FILE CONTENT:1840 - 4 Jul 2004 VOL 141 ISS 1

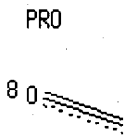
****
*
* CASREACT now has more than 8 million reactions
*
****

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

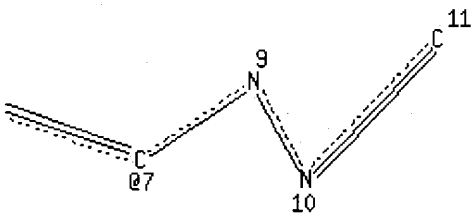
This file contains CAS Registry Numbers for easy and accurate substance identification.

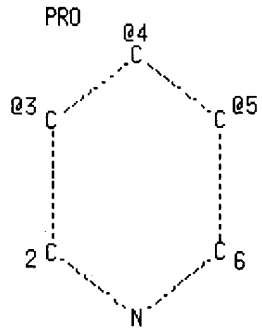
=>
L4 STRUCTURE UPLOADED

=> d 14
L4 HAS NO ANSWERS
L4 STR
0 24 S 25

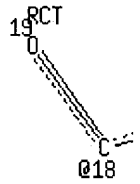


Page 1-A





Page 1-B



Page 2-A

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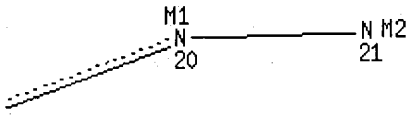
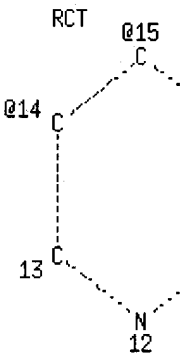
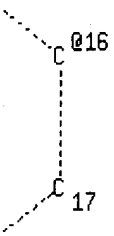


RCT
22

Page 2-B



Page 3-A



Page 3-B
VAR G1=24/25
VPA 7-3/4/5 S
VPA 18-14/15/16 S
NODE ATTRIBUTES:

```
HCOUNT   IS M1      AT  20
HCOUNT   IS M2      AT  21
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS C       AT   7
NSPEC    IS C       AT   8
NSPEC    IS C       AT   9
NSPEC    IS C       AT  10
NSPEC    IS RC      AT  11
NSPEC    IS R       AT  12
NSPEC    IS R       AT  13
NSPEC    IS R       AT  14
NSPEC    IS R       AT  15
NSPEC    IS R       AT  16
NSPEC    IS R       AT  17
NSPEC    IS C       AT  18
NSPEC    IS C       AT  19
NSPEC    IS C       AT  20
NSPEC    IS C       AT  21
NSPEC    IS C       AT  22
NSPEC    IS RC      AT  23
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS   AT   7  8  9 10 11 18 19 20 21 23 24 25
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE


=> s l4
SAMPLE SEARCH INITIATED 15:45:45 FILE 'CASREACT'
SCREENING COMPLETE -    147 REACTIONS TO VERIFY FROM     27 DOCUMENTS

100.0% DONE    147 VERIFIED      53 HIT RXNS                    11 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:      2213 TO     3667
PROJECTED ANSWERS:              22 TO      418

L5            11 SEA SSS SAM L4 (    53 REACTIONS)

=> s l4 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:45:49 FILE 'CASREACT'
SCREENING COMPLETE -   3426 REACTIONS TO VERIFY FROM    643 DOCUMENTS

100.0% DONE   3426 VERIFIED     618 HIT RXNS                   187 DOCS
SEARCH TIME: 00.00.01

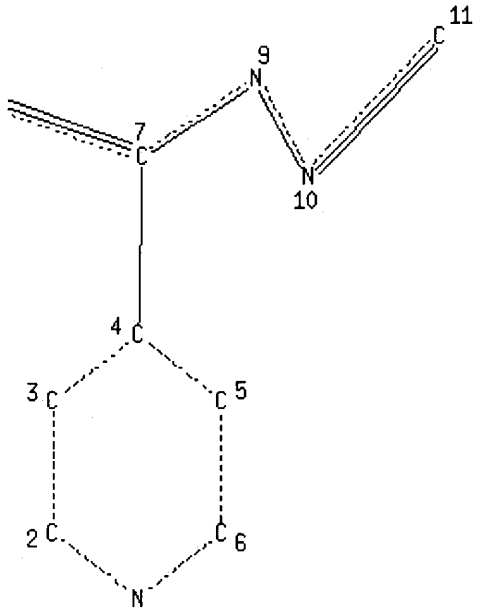
L6           187 SEA SSS FUL L4 (   618 REACTIONS)
```

```
=>
L7       STRUCTURE UPLOADED

=> d 17
L7 HAS NO ANSWERS
L7                 STR
 0 24 S 25
```

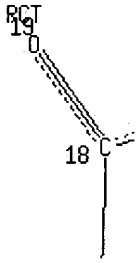
PRO

Page 1-A



Page 1-B

RCT



Page 2-A

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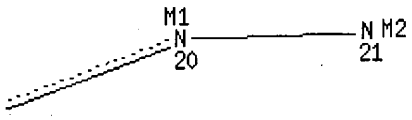
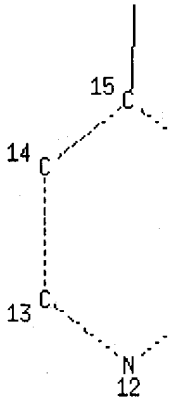
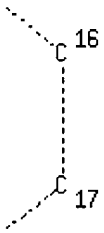


RCT
22

Page 2-B



Page 3-A



Page 3-B

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VAR G1=24/25
NODE ATTRIBUTES:
HCOUNT   IS M1      AT  20
HCOUNT   IS M2      AT  21
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
```

```
NSPEC   IS R      AT   6
NSPEC   IS C      AT   7
NSPEC   IS C      AT   8
NSPEC   IS C      AT   9
NSPEC   IS C      AT  10
NSPEC   IS RC     AT  11
NSPEC   IS R      AT  12
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NSPEC   IS R      AT  16
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NSPEC   IS C      AT  19
NSPEC   IS C      AT  20
NSPEC   IS C      AT  21
NSPEC   IS C      AT  22
NSPEC   IS RC     AT  23
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8  9 10 11 18 19 20 21 23 24 25
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  25

STEREO ATTRIBUTES: NONE


=> s l7
SAMPLE SEARCH INITIATED 15:47:23 FILE 'CASREACT'
SCREENING COMPLETE -     50 REACTIONS TO VERIFY FROM     13 DOCUMENTS

100.0% DONE     50 VERIFIED      24 HIT RXNS                      10 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:       576 TO     1424
PROJECTED ANSWERS:              11 TO      389

L8            10 SEA SSS SAM L7 (    24 REACTIONS)

=> s l7 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:47:28 FILE 'CASREACT'
SCREENING COMPLETE -    957 REACTIONS TO VERIFY FROM    233 DOCUMENTS

100.0% DONE    957 VERIFIED     443 HIT RXNS                     157 DOCS
SEARCH TIME: 00.00.01

L9          157 SEA SSS FUL L7 (   443 REACTIONS)

=> file reg
COST IN U.S. DOLLARS                            SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               209.64     224.82

FILE 'REGISTRY' ENTERED AT 15:47:49 ON 09 JUL 2004
```

```
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provided by InfoChem.

STRUCTURE FILE UPDATES:    8 JUL 2004  HIGHEST RN 706430-72-0
DICTIONARY FILE UPDATES:   8 JUL 2004  HIGHEST RN 706430-72-0

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 6, 2004

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

Crossover limits have been increased.  See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=> e absolute ethanol/cn
E1            1     ABSOLAC SP 200/CN
E2            1     ABSOLUTE/CN
E3            0 --> ABSOLUTE ETHANOL/CN
E4            1     ABSON/CN
E5            1     ABSON 69163/CN
E6            1     ABSON 820X14/CN
E7            1     ABSON 820X17/CN
E8            1     ABSON 821/CN
E9            1     ABSON 89110/CN
E10           1     ABSON 89120/CN
E11           1     ABSON 89131/CN
E12           1     ABSON 89140/CN

=> file casreact
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                               0.42     225.24

FILE 'CASREACT' ENTERED AT 15:48:05 ON 09 JUL 2004
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for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 4 Jul 2004 VOL 141 ISS 1

************************************************************
*                                                          *
*     CASREACT now has more than  8 million reactions      *
*                                                          *
************************************************************

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991)
provided by InfoChem, INPI data prior to 1986, and Biotransformations
```
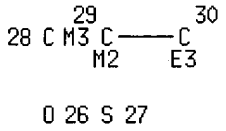

database compiled under the direction of Professor Dr. Klaus Kieslich.

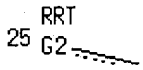
This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
L10 STRUCTURE UPLOADED

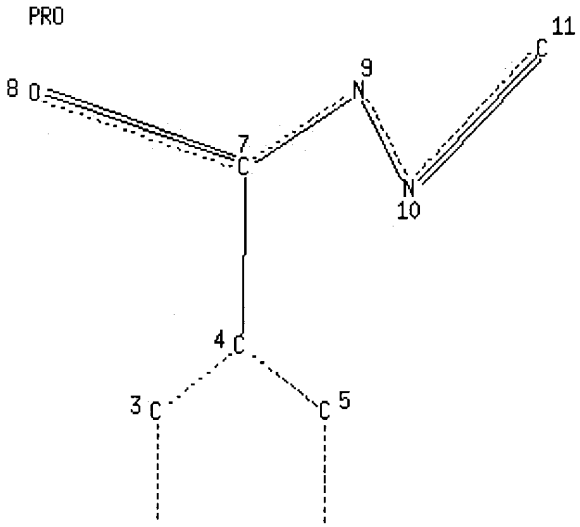
=> d l10
L10 HAS NO ANSWERS
L10 STR



0 26 S 27



Page 1-C



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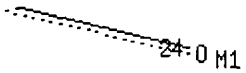

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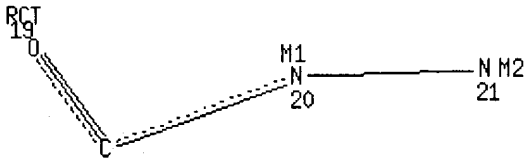

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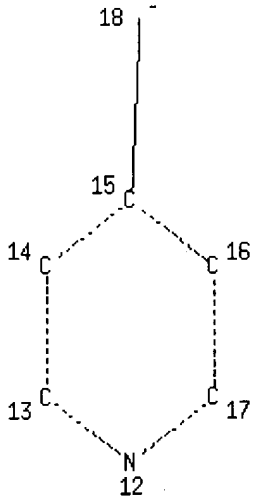
Page 3-A



Page 3-D
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VAR G2=28/29
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HCOUNT   IS M2      AT  21
HCOUNT   IS M1      AT  24
HCOUNT   IS M3      AT  28
HCOUNT   IS M2      AT  29
HCOUNT   IS E3      AT  30
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS C       AT   7
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NSPEC    IS RC      AT  11
NSPEC    IS R       AT  12
NSPEC    IS R       AT  13
NSPEC    IS R       AT  14
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NSPEC    IS C       AT  22
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MLEVEL   IS CLASS  AT   7  8  9 10 11 18 19 20 21 23 24 26 27 28 29 30
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  30

STEREO ATTRIBUTES: NONE


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SAMPLE SEARCH INITIATED 15:50:55 FILE 'CASREACT'
SCREENING COMPLETE -     50 REACTIONS TO VERIFY FROM     13 DOCUMENTS

100.0% DONE     50 VERIFIED       6 HIT RXNS                      1 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:       576 TO     1424
PROJECTED ANSWERS:               1 TO       79

L11            1 SEA SSS SAM L10 (     6 REACTIONS)

=> s l11 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:51:02 FILE 'CASREACT'
SCREENING COMPLETE -    956 REACTIONS TO VERIFY FROM    232 DOCUMENTS
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100.0% DONE    956 VERIFIED       9 HIT RXNS                    3 DOCS
SEARCH TIME: 00.00.01

L12           3 SEA SSS FUL L10 (     9 REACTIONS)

=> d l12, crd rxn ibib abs, 1-3
'RXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS -------- GI and AB
ALL -------- BIB, AB, IND, RE, Single-step Reactions
APPS ------- AI, PRAI
BIB -------- AN, plus Bibliographic Data
CAN -------- List of CA abstract numbers without answer numbers
CBIB ------- AN, plus Compressed Bibliographic Data
DALL ------- ALL, delimited (end of each field identified)
IABS ------- ABS, indented with text labels
IALL ------- ALL, indented with text labels
IBIB ------- BIB, indented with text labels
IND -------- Indexing data
IPC -------- International Patent Classifications
ISTD ------- STD, indented with text labels
OBIB -------- AN, plus Bibliographic Data (original)
OIBIB ------- OBIB, indented with text labels

SBIB -------- BIB, no citations
SIBIB ------- IBIB, no citations

MAX -------- Same as ALL
PATS ------- PI, SO
SCAN ------- TI and FCRD (random display, no answer number.  SCAN
             must be entered on the same line as DISPLAY, e.g.,
             D SCAN.)
SSRX ------- Single-Step Reactions (Map, Diagram, and Summary for
             all single-step reactions)
STD -------- BIB, IPC, and NCL

CRD -------- Compact Display of All Hit Reactions
CRDREF ----- Compact Reaction Display and SO, PY for Reference
FHIT ------- Reaction Map, Diagram, and Summary for first
             hit reaction
FHITCBIB --- FHIT, AN plus CBIB
FCRD ------- First hit in Compact Reaction Display (CRD) format
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with
             CA reference information (SO, PY).  (Default)
FPATH ------ PATH, plus Reaction Summary for the "long path"
FSPATH ----- SPATH, plus Reaction Summary for the "short path"
HIT -------- Reaction Map, Reaction Diagram, and Reaction
             Summary for all hit reactions and fields containing
             hit terms
OCC -------- All hit fields and the number of occurrences of the
             hit terms in each field.  Includes total number of
             HIT, PATH, SPATH reactions. Labels reactions that have
             incomplete verifications.
PATH ------- Reaction Map and Reaction Diagram for the "long
             path".  Displays all hit reactions, except those
             whose steps are totally included within another hit
             reaction which is displayed
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```
RX --------- Hit Reactions (Map, Diagram, Summary for all hit reactions)
RXG -------- Hit Reaction Graphics (Map and Diagram for all hit reactions)
RXL -------- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)
RXS -------- Hit Reaction Summariers (Map and Summary for all hit reactions)
SPATH ------ Reaction Map and Reaction Diagram for the "short
             path". Displays all single step reactions which
             contain a hit substance. Also displays those
             multistep reactions that have a hit substance in both
             the first and last steps of the reaction, except for
             those hit reactions whose steps are totally included
             within another hit reaction which is displayed

To display a particular field or fields, enter the display field
codes. For a list of the display field codes, enter HELP DFIELDS
at an arrow prompt (=>). Examples of combinations include: D TI;
D BIB RX; D TI, AU, FCRD. The information is displayed in the same order
as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may
be used with the DISPLAY command to display the record for a specified
Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

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     (FILE 'HOME' ENTERED AT 15:26:37 ON 09 JUL 2004)

     FILE 'REGISTRY' ENTERED AT 15:26:43 ON 09 JUL 2004
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L1            1 S E3
                E 310427-65-7/RN
L2            1 S E3
                E 10325-94-7/RN
L3            1 S E3

     FILE 'CASREACT' ENTERED AT 15:40:30 ON 09 JUL 2004
L4              STRUCTURE UPLOADED
L5           11 S L4
L6          187 S L4 FULL
L7              STRUCTURE UPLOADED
L8           10 S L7
L9          157 S L7 FULL

     FILE 'REGISTRY' ENTERED AT 15:47:49 ON 09 JUL 2004
                E ABSOLUTE ETHANOL/CN

     FILE 'CASREACT' ENTERED AT 15:48:05 ON 09 JUL 2004
L10             STRUCTURE UPLOADED
L11           1 S L10
L12           3 S L11 FULL

=> d l12, ibib abs fhit abs, 1-3


L12  ANSWER 1 OF 3  CASREACT  COPYRIGHT 2004 ACS on STN
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Full Text | Citing References

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ACCESSION NUMBER:         138:39232  CASREACT
TITLE:                    Synthesis and biological activity of some
                          1,2,4-triazoles and related heterocycles
```
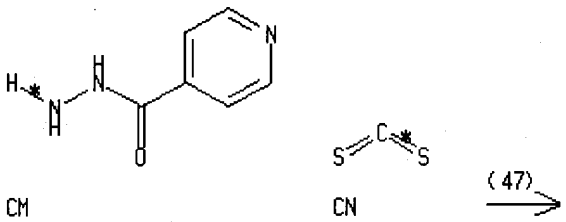
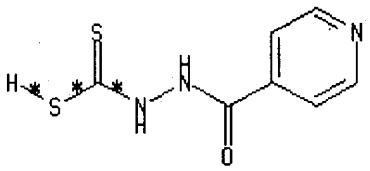

AUTHOR(S): Udupi, R. H.; Kulkarni, V. M.; Sudheendra; Setty, S. Ramachandra; Purushottamachar, P.
CORPORATE SOURCE: Department of Pharmaceutical Chemistry, V.L. College of Pharmacy, Raichur, 584 101, India
SOURCE: Indian Journal of Heterocyclic Chemistry (2002), 11(4), 303-308
CODEN: IJCHEI; ISSN: 0971-1627
PUBLISHER: Prof. R. S. Varma
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 4-Amino-2,4-dihydro-5-(4-pyridinyl)-3H-1,2,4-triazole-3-thione and 5-(4-pyridinyl)-4-[[(4-pyridinyl)carbonyl]amino]-3H-1,2,4-triazole-3-thione were prepd.; cyclocondensation of the latter with aryl carboxylic acids or aryl aldehydes gave 6-aryl-3-(4-pyridinyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole derivs. Some of them were found to be potential antiinflammatory and antimicrobial agents.

RX(47) OF 143 **CM** + **CN** ===> **CO**...



CM CN



K

CO

RX(47) RCT CM **54-85-3**, CN **75-15-0**
RGT CP 1310-58-3 KOH, CQ **64-17-5** EtOH, BM 7732-18-5 Water
PRO CO **61019-32-7**
AB 4-Amino-2,4-dihydro-5-(4-pyridinyl)-3H-1,2,4-triazole-3-thione and 5-(4-pyridinyl)-4-[[(4-pyridinyl)carbonyl]amino]-3H-1,2,4-triazole-3-thione were prepd.; cyclocondensation of the latter with aryl carboxylic acids or aryl aldehydes gave 6-aryl-3-(4-pyridinyl)-1,2,4-triazolo[3,4-b][1,3,4]thiadiazole derivs. Some of them were found to be potential antiinflammatory and antimicrobial agents.
REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L12 ANSWER 2 OF 3 CASREACT COPYRIGHT 2004 ACS on STN
Full Text | Citing References
ACCESSION NUMBER: 135:131724 CASREACT
TITLE: Synthesis and structure-activity relationships of

potent and orally active sulfonamide ETB selective antagonists

AUTHOR(S): Kanda, Y.; Kawanishi, Y.; Oda, K.; Sakata, T.; Mihara, S.; Asakura, K.; Kanemasa, T.; Ninomiya, M.; Fujimoto, M.; Konoike, T.

CORPORATE SOURCE: Shionogi Research Laboratories, Shionogi & Co., Ltd., Fukushima-ku, Osaka, 553-0002, Japan

SOURCE: Bioorganic & Medicinal Chemistry (2001), 9(4), 897-907
CODEN: BMECEP; ISSN: 0968-0896

PUBLISHER: Elsevier Science Ltd.

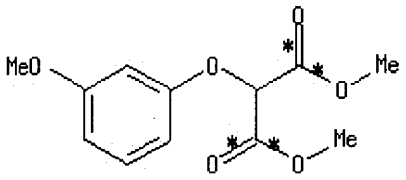
DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis and structure-activity relationships of a series of N-pyrimidinyl benzenesulfonamides as ETB selective antagonists are described. N-Isoxazolyl benzenesulfonamide (I), previously reported, was selected as a lead compd., and isosteric replacement of the isoxazole ring of I with a pyrimidine ring led to the discovery of a highly potent ETB selective antagonist with oral bioavailability. Modification of the terminal aldehyde group at the 6-position of the pyrimidine ring was investigated, and malonate and acylhydrazone derivs. were equipotent to aldehyde deriv. (II). Compd. II showed ETB antagonistic activity on in vivo evaluation.

RX(120) OF 135 COMPOSED OF RX(29), RX(2), RX(3), RX(4), RX(30), RX(27)

RX(120) **C** + AG + J + M + **BT** ===> **BU**



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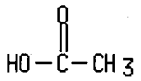

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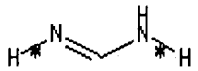

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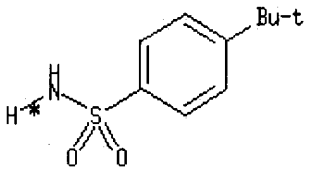

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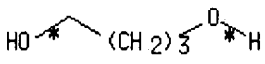

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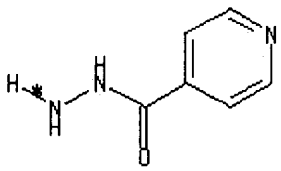
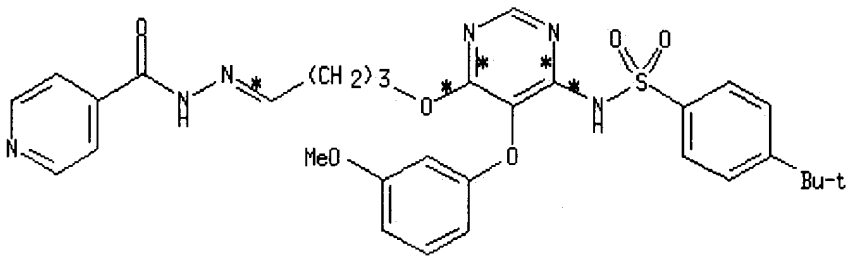


BT

6
STEPS



BU

RX(29) RCT C **189574-46-7**, AG 3473-63-0
RGT D **124-41-4** NaOMe
PRO F 202288-10-6
SOL 67-56-1 MeOH

RX(2) RCT F 202288-10-6
RGT H 10025-87-3 POCl3
PRO G 150727-28-9
SOL 10025-87-3 POCl3, 108-75-8 s-Collidine

RX(3) RCT G 150727-28-9, J 146796-98-7
PRO K 150727-29-0
SOL 67-68-5 DMSO

RX(4) RCT K 150727-29-0, M 110-63-4
RGT O 7646-69-7 NaH
PRO N 202288-11-7
SOL 110-63-4 HO(CH2)4OH

RX(30) RCT N 202288-11-7
RGT R 26299-14-9 PCC
PRO AO 202287-80-7
SOL 75-09-2 CH2Cl2

RX(27) RCT AO 202287-80-7, BT **54-85-3**
PRO BU **231613-18-6**
SOL 64-17-5 EtOH

AB The synthesis and structure-activity relationships of a series of N-pyrimidinyl benzenesulfonamides as ETB selective antagonists are described. N-Isoxazolyl benzenesulfonamide (I), previously reported, was selected as a lead compd., and isosteric replacement of the isoxazole ring of I with a pyrimidine ring led to the discovery of a highly potent ETB selective antagonist with oral bioavailability. Modification of the terminal aldehyde group at the 6-position of the pyrimidine ring was investigated, and malonate and acylhydrazone derivs. were equipotent to aldehyde deriv. (II). Compd. II showed ETB antagonistic activity on in vivo evaluation.

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

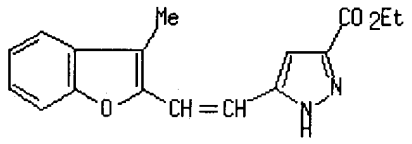
L12 ANSWER 3 OF 3 CASREACT COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 104:50817 CASREACT
TITLE: Synthesis of nitrogenous compounds from δ-unsaturated 1,3-dicarbonyl esters: trisubstituted pyrazoles of possible antimicrobial and

hypoglycemic activities and hydrazones with antituberculosis activity

AUTHOR(S): Mokhtar, Hassan M.; Wojtanis, J.
CORPORATE SOURCE: Fac. Sci., Alexandria Univ., Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1985), 24B(2), 188-92
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



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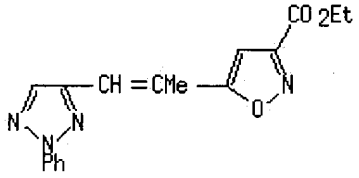
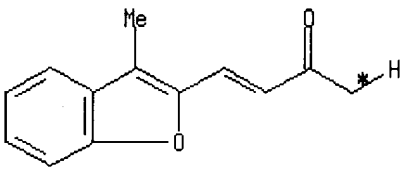


IV

AB R1CH:CRCOCH2COCO2Et (I, R = H, Me, Ph; R1 = 3-methylbenzofuran-2-yl, 2-phenyl-2H-1,2,3-triazol-4-yl) were prepd. by condensing R1CH:CRCOMe (II) with Et oxalate in dry ether. Treating I with hydrazine and arylhydrazines caused cyclization to the corresponding Et substituted pyrazole-3-carboxylates, e.g., III, which were hydrolyzed to acids or converted into acid hydrazides. Condensing I with acylhydrazines gave hydrazones which were cyclized to the corresponding N-acylpyrazoles. Treating I with HONH2 gave 3,5-disubstituted isoxazoles, e.g., IV, whereas using o-phenylenediamine gave hydroxyquinoxalines. Reaction of II with arylhydrazines gave the corresponding hydrazones, which on boiling with EtOH-HCl cyclized to pyrazolines. Treating the latter compds. with excess bromine-water gave the brominated pyrazoles. Condensing II with acylhydrazines gave the corresponding acylhydrazones.

RX(167) OF 375 COMPOSED OF RX(6), RX(85)
RX(167) **C** + N + **DQ** ===> **DR**



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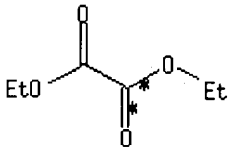

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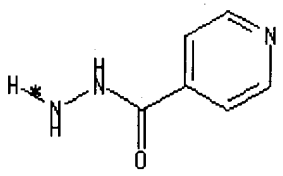
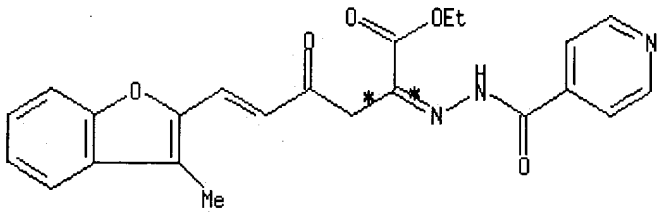


DQ

2 STEPS



DR

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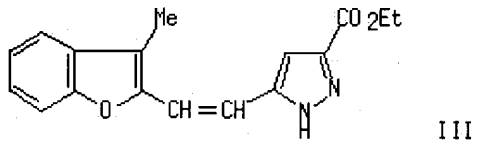
RGT P **141-52-6** NaOEt
PRO O 99410-72-7
SOL 71-43-2 Benzene, 60-29-7 Et2O

RX(85) RCT DQ **54-85-3**, O 99410-72-7
RGT DB 64-19-7 AcOH
PRO DR **99411-45-7**
SOL 64-17-5 EtOH

GI



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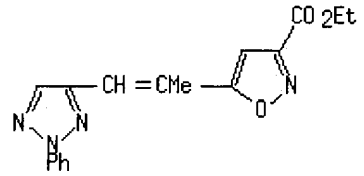

IV

AB R1CH:CRCOCH2COCO2Et (I, R = H, Me, Ph; R1 = 3-methylbenzofuran-2-yl, 2-phenyl-2H-1,2,3-triazol-4-yl) were prepd. by condensing R1CH:CRCOMe (II) with Et oxalate in dry ether. Treating I with hydrazine and arylhydrazines caused cyclization to the corresponding Et substituted pyrazole-3-carboxylates, e.g., III, which were hydrolyzed to acids or converted into acid hydrazides. Condensing I with acylhydrazines gave hydrazones which were cyclized to the corresponding N-acylpyrazoles. Treating I with HONH2 gave 3,5-disubstituted isoxazoles, e.g., IV, whereas using o-phenylenediamine gave hydroxyquinoxalines. Reaction of II with arylhydrazines gave the corresponding hydrazones, which on boiling with EtOH-HCl cyclized to pyrazolines. Treating the latter compds. with excess bromine-water gave the brominated pyrazoles. Condensing II with acylhydrazines gave the corresponding acylhydrazones.

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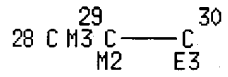

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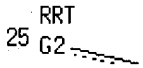
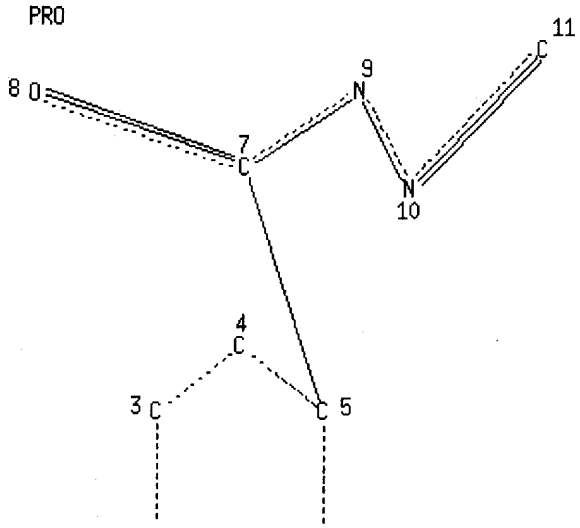
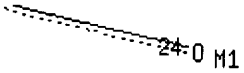


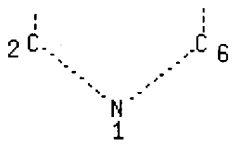
Page 1-C

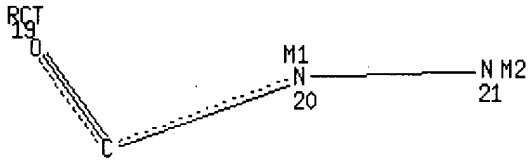


Page 1-D

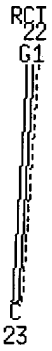


Page 2-C

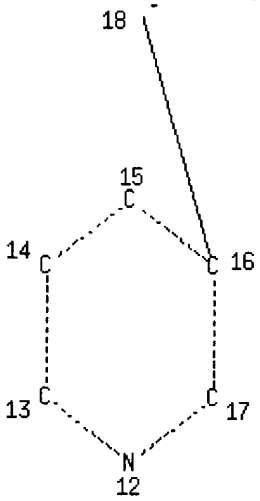




Page 2-D



Page 3-A



Page 3-D
VAR G1=26/27
VAR G2=28/29
NODE ATTRIBUTES:
HCOUNT IS M1 AT 20

```
HCOUNT   IS M2      AT  21
HCOUNT   IS M1      AT  24
HCOUNT   IS M3      AT  28
HCOUNT   IS M2      AT  29
HCOUNT   IS E3      AT  30
NSPEC    IS R       AT   1
NSPEC    IS R       AT   2
NSPEC    IS R       AT   3
NSPEC    IS R       AT   4
NSPEC    IS R       AT   5
NSPEC    IS R       AT   6
NSPEC    IS C       AT   7
NSPEC    IS C       AT   8
NSPEC    IS C       AT   9
NSPEC    IS C       AT  10
NSPEC    IS RC      AT  11
NSPEC    IS R       AT  12
NSPEC    IS R       AT  13
NSPEC    IS R       AT  14
NSPEC    IS R       AT  15
NSPEC    IS R       AT  16
NSPEC    IS R       AT  17
NSPEC    IS C       AT  18
NSPEC    IS C       AT  19
NSPEC    IS C       AT  20
NSPEC    IS C       AT  21
NSPEC    IS C       AT  22
NSPEC    IS RC      AT  23
NSPEC    IS C       AT  24
NSPEC    IS C       AT  25
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS  AT   7  8  9 10 11 18 19 20 21 23 24 26 27 28 29 30
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  30

STEREO ATTRIBUTES: NONE


=> s l13
SAMPLE SEARCH INITIATED 15:55:44 FILE 'CASREACT'
SCREENING COMPLETE -     33 REACTIONS TO VERIFY FROM      7 DOCUMENTS

100.0% DONE     33 VERIFIED       6 HIT RXNS                      1 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:       316 TO     1004
PROJECTED ANSWERS:               1 TO       79

L14            1 SEA SSS SAM L13 (     6 REACTIONS)

=> s l13 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:55:53 FILE 'CASREACT'
SCREENING COMPLETE -     419 REACTIONS TO VERIFY FROM     77 DOCUMENTS
```

100.0% DONE 419 VERIFIED 6 HIT RXNS 1 DOCS
SEARCH TIME: 00.00.01

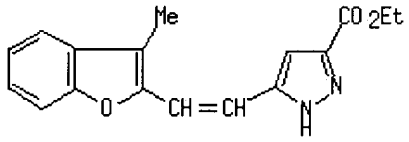
L15 1 SEA SSS FUL L13 (6 REACTIONS)

=> d l15, ibib abs fhit, 1

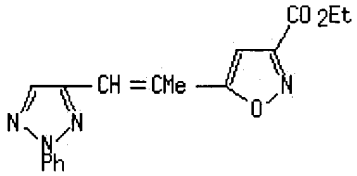
L15 ANSWER 1 OF 1 CASREACT COPYRIGHT 2004 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 104:50817 CASREACT
TITLE: Synthesis of nitrogenous compounds from δ-unsaturated 1,3-dicarbonyl esters: trisubstituted pyrazoles of possible antimicrobial and hypoglycemic activities and hydrazones with antituberculosis activity
AUTHOR(S): Mokhtar, Hassan M.; Wojtanis, J.
CORPORATE SOURCE: Fac. Sci., Alexandria Univ., Egypt
SOURCE: Indian Journal of Chemistry, Section B: Organic Chemistry Including Medicinal Chemistry (1985), 24B(2), 188-92
CODEN: IJSBDB; ISSN: 0376-4699
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



III

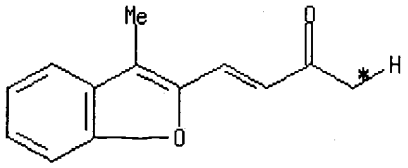


IV

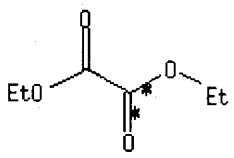
AB R1CH:CRCOCH2COCO2Et (I, R = H, Me, Ph; R1 = 3-methylbenzofuran-2-yl, 2-phenyl-2H-1,2,3-triazol-4-yl) were prepd. by condensing R1CH:CRCOMe (II) with Et oxalate in dry ether. Treating I with hydrazine and arylhydrazines caused cyclization to the corresponding Et substituted pyrazole-3-carboxylates, e.g., III, which were hydrolyzed to acids or converted into acid hydrazides. Condensing I with acylhydrazines gave hydrazones which were cyclized to the corresponding N-acylpyrazoles. Treating I with HONH2 gave 3,5-disubstituted isoxazoles, e.g., IV, whereas using o-phenylenediamine gave hydroxyquinoxalines. Reaction of II with arylhydrazines gave the corresponding hydrazones, which on boiling with EtOH-HCl cyclized to pyrazolines. Treating the latter compds. with excess bromine-water gave the brominated pyrazoles. Condensing II with acylhydrazines gave the corresponding acylhydrazones.

RX(168) OF 375 COMPOSED OF RX(6), RX(86)

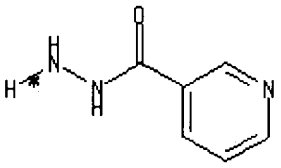
RX(168) **C** + N + **DS** ===> **DT**



C

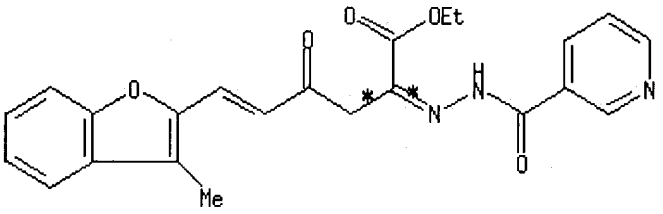


N



DS

2 STEPS



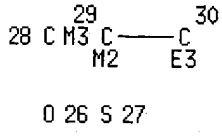
DT

RX(6) RCT C **99410-65-8**, N 95-92-1
RGT P **141-52-6** NaOEt
PRO O 99410-72-7
SOL 71-43-2 Benzene, 60-29-7 Et2O

RX(86) RCT DS **553-53-7**, O 99410-72-7
RGT DB 64-19-7 AcOH
PRO DT **99411-46-8**
SOL 64-17-5 EtOH

=>
L16 STRUCTURE UPLOADED

=> d l16
L16 HAS NO ANSWERS
L16 STR



0 26 S 27

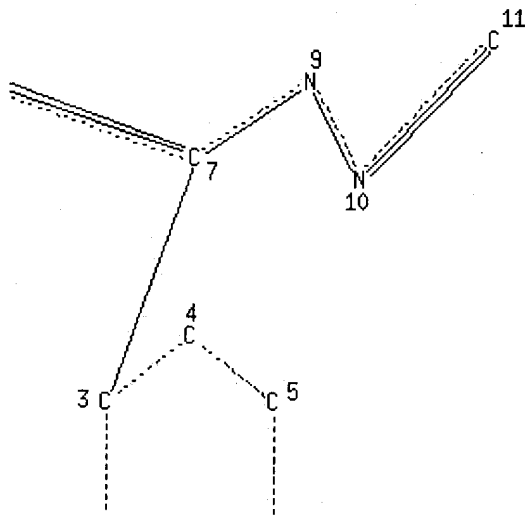
PRO

8 O

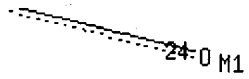
RRT

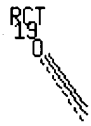
25 G2

Page 1-A

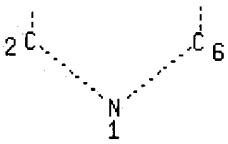


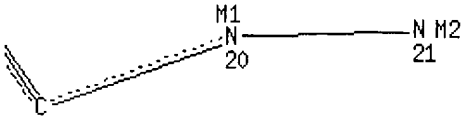
Page 1-B



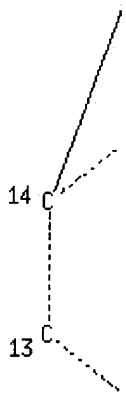


Page 2-A

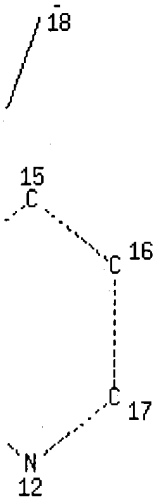




Page 2-B



Page 3-A



Page 3-B

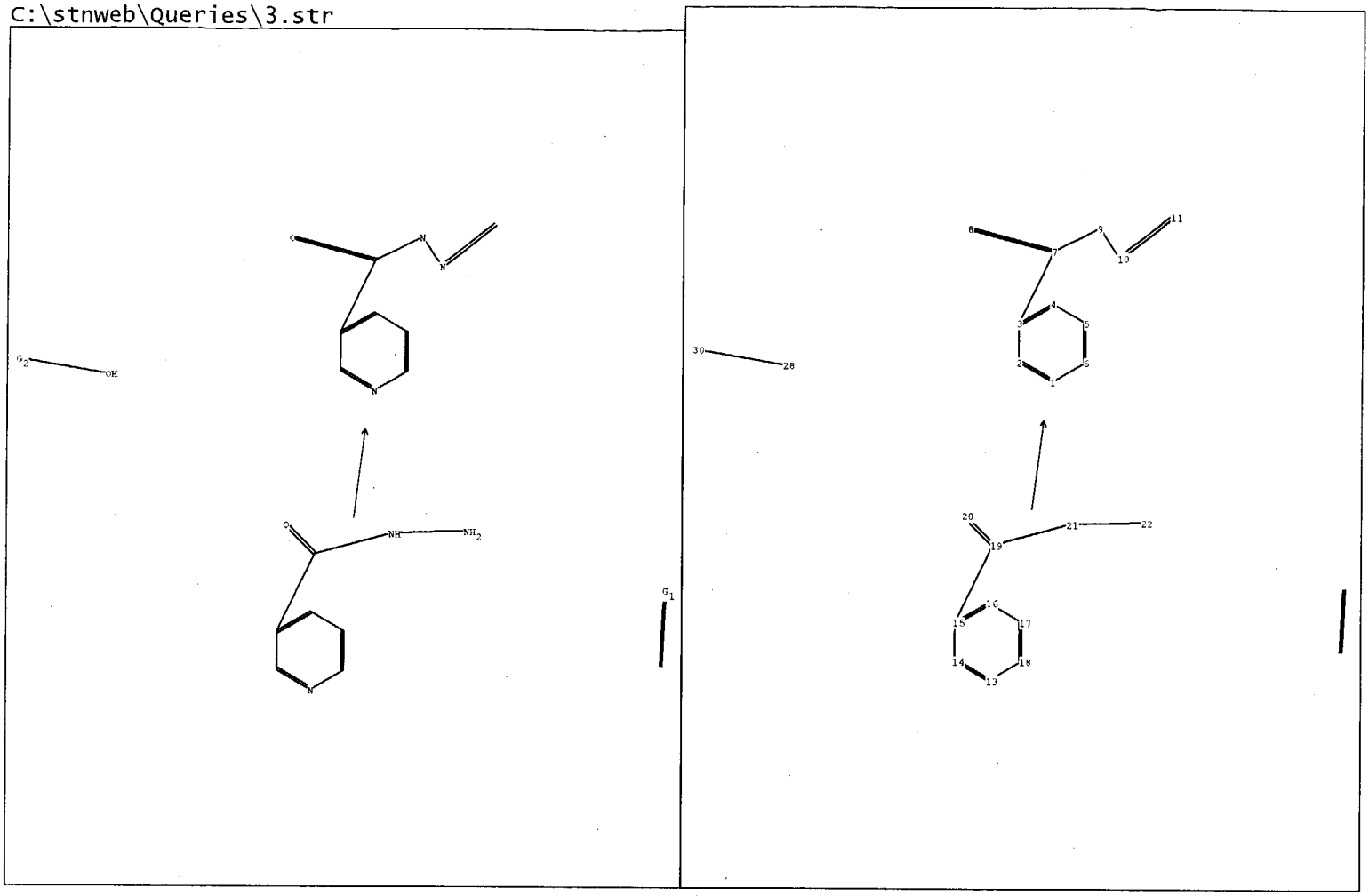
```
VAR G1=26/27
VAR G2=28/29
NODE ATTRIBUTES:
HCOUNT  IS M1     AT  20
HCOUNT  IS M2     AT  21
HCOUNT  IS M1     AT  24
HCOUNT  IS M3     AT  28
HCOUNT  IS M2     AT  29
HCOUNT  IS E3     AT  30
NSPEC   IS R      AT   1
NSPEC   IS R      AT   2
NSPEC   IS R      AT   3
NSPEC   IS R      AT   4
NSPEC   IS R      AT   5
NSPEC   IS R      AT   6
NSPEC   IS C      AT   7
NSPEC   IS C      AT   8
NSPEC   IS C      AT   9
NSPEC   IS C      AT  10
NSPEC   IS RC     AT  11
NSPEC   IS R      AT  12
NSPEC   IS R      AT  13
NSPEC   IS R      AT  14
NSPEC   IS R      AT  15
NSPEC   IS R      AT  16
NSPEC   IS R      AT  17
```

```
NSPEC   IS C      AT  18
NSPEC   IS C      AT  19
NSPEC   IS C      AT  20
NSPEC   IS C      AT  21
NSPEC   IS C      AT  22
NSPEC   IS RC     AT  23
NSPEC   IS C      AT  24
NSPEC   IS C      AT  25
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8  9 10 11 18 19 20 21 23 24 26 27 28 29 30
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  30

STEREO ATTRIBUTES: NONE


=> s l16
SAMPLE SEARCH INITIATED 15:58:58 FILE 'CASREACT'
SCREENING COMPLETE -     33 REACTIONS TO VERIFY FROM      7 DOCUMENTS

100.0% DONE     33 VERIFIED       6 HIT RXNS                     1 DOCS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED VERIFICATIONS:       316 TO     1004
PROJECTED ANSWERS:               1 TO       79

L17           1 SEA SSS SAM L16 (     6 REACTIONS)

=> s l16 full
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 102.30 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 15:59:05 FILE 'CASREACT'
SCREENING COMPLETE -    419 REACTIONS TO VERIFY FROM     77 DOCUMENTS

100.0% DONE    419 VERIFIED       6 HIT RXNS                     1 DOCS
SEARCH TIME: 00.00.01

L18           1 SEA SSS FUL L16 (     6 REACTIONS)

=> d his

     (FILE 'HOME' ENTERED AT 15:26:37 ON 09 JUL 2004)

     FILE 'REGISTRY' ENTERED AT 15:26:43 ON 09 JUL 2004
                E  310427-67-9/RN
L1            1 S E3
                E 310427-65-7/RN
L2            1 S E3
                E 10325-94-7/RN
L3            1 S E3

     FILE 'CASREACT' ENTERED AT 15:40:30 ON 09 JUL 2004
L4              STRUCTURE UPLOADED
L5           11 S L4
L6          187 S L4 FULL
```

```
L7              STRUCTURE UPLOADED
L8           10 S L7
L9          157 S L7 FULL

     FILE 'REGISTRY' ENTERED AT 15:47:49 ON 09 JUL 2004
                E ABSOLUTE ETHANOL/CN

     FILE 'CASREACT' ENTERED AT 15:48:05 ON 09 JUL 2004
L10             STRUCTURE UPLOADED
L11           1 S L10
L12           3 S L11 FULL
L13             STRUCTURE UPLOADED
L14           1 S L13
L15           1 S L13 FULL
L16             STRUCTURE UPLOADED
L17           1 S L16
L18           1 S L16 FULL

=> s l18 not l15
L19           0 L18 NOT L15
```

containing 28

C:\stnweb\Queries\3.str



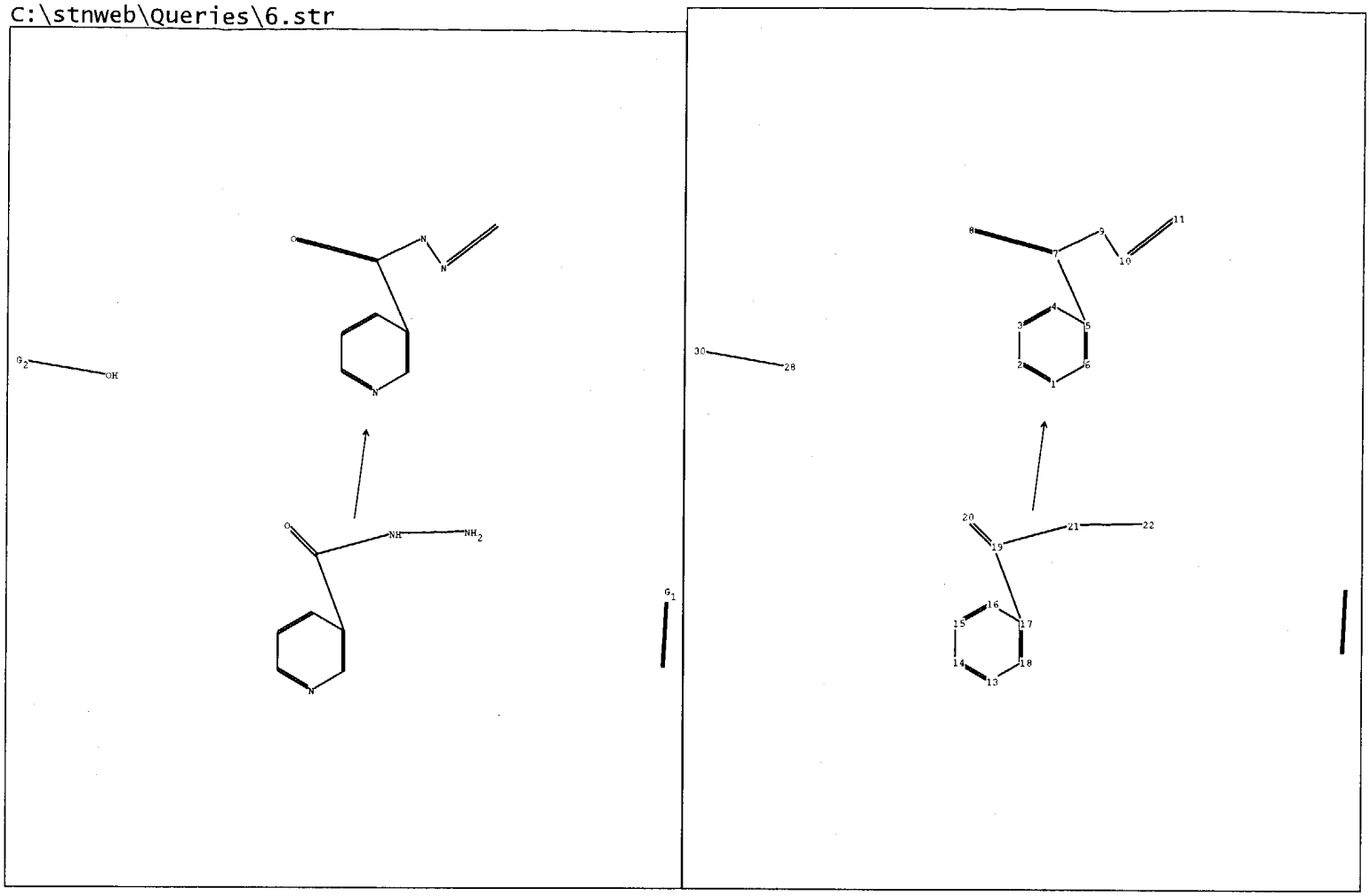
chain nodes :
7 8 9 10 19 20 21 22 24 28 30
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
ring/chain nodes :
11 25
chain bonds :
3-7 7-9 7-8 9-10 10-11 15-19 19-21 19-20 21-22 24-25 28-30
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
7-9 7-8 9-10 10-11 19-21 19-20 24-25 28-30
exact bonds :
3-7 15-19 21-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
isolated ring systems :
containing 1 : 13 :

G1:O,S

G2:CH3,Et

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:CLASS 24:CLASS 25:CLASS 28:CLASS 30:CLASS
fragments assigned reactant role:
containing 13
containing 24
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:

C:\stnweb\Queries\6.str



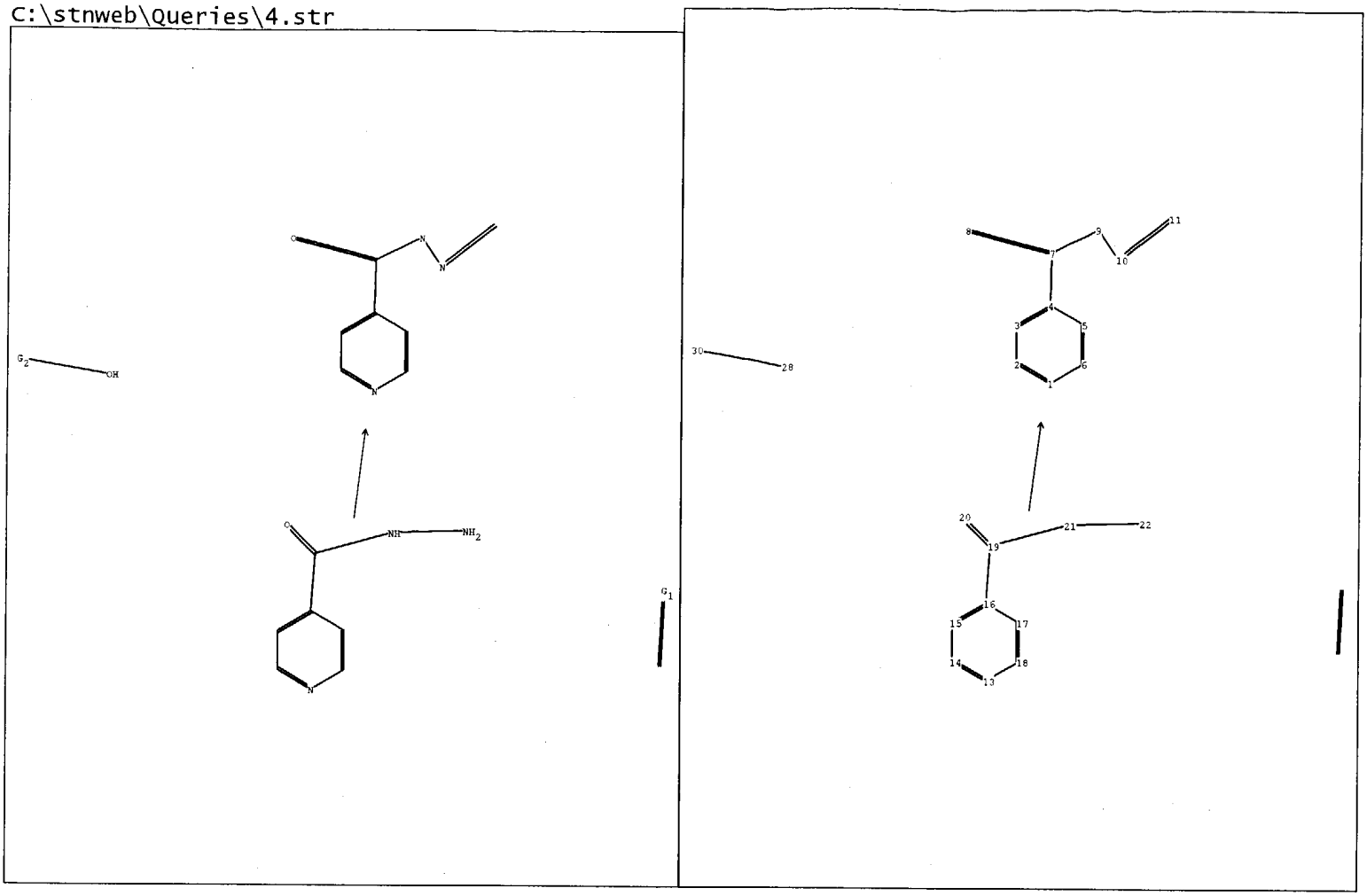
chain nodes :
7 8 9 10 19 20 21 22 24 28 30
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
ring/chain nodes :
11 25
chain bonds :
5-7 7-9 7-8 9-10 10-11 17-19 19-21 19-20 21-22 24-25 28-30
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
7-9 7-8 9-10 10-11 19-21 19-20 24-25 28-30
exact bonds :
5-7 17-19 21-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
isolated ring systems :
containing 1 : 13 :

G1:O,S

G2:CH3,Et

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:CLASS 24:CLASS 25:CLASS 28:CLASS 30:CLASS
fragments assigned reactant role:
containing 13
containing 24
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:

C:\stnweb\Queries\4.str



chain nodes :
7 8 9 10 19 20 21 22 24 28 30
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
ring/chain nodes :
11 25
chain bonds :
4-7 7-9 7-8 9-10 10-11 16-19 19-21 19-20 21-22 24-25 28-30
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
7-9 7-8 9-10 10-11 19-21 19-20 24-25 28-30
exact bonds :
4-7 16-19 21-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
isolated ring systems :
containing 1 : 13 :

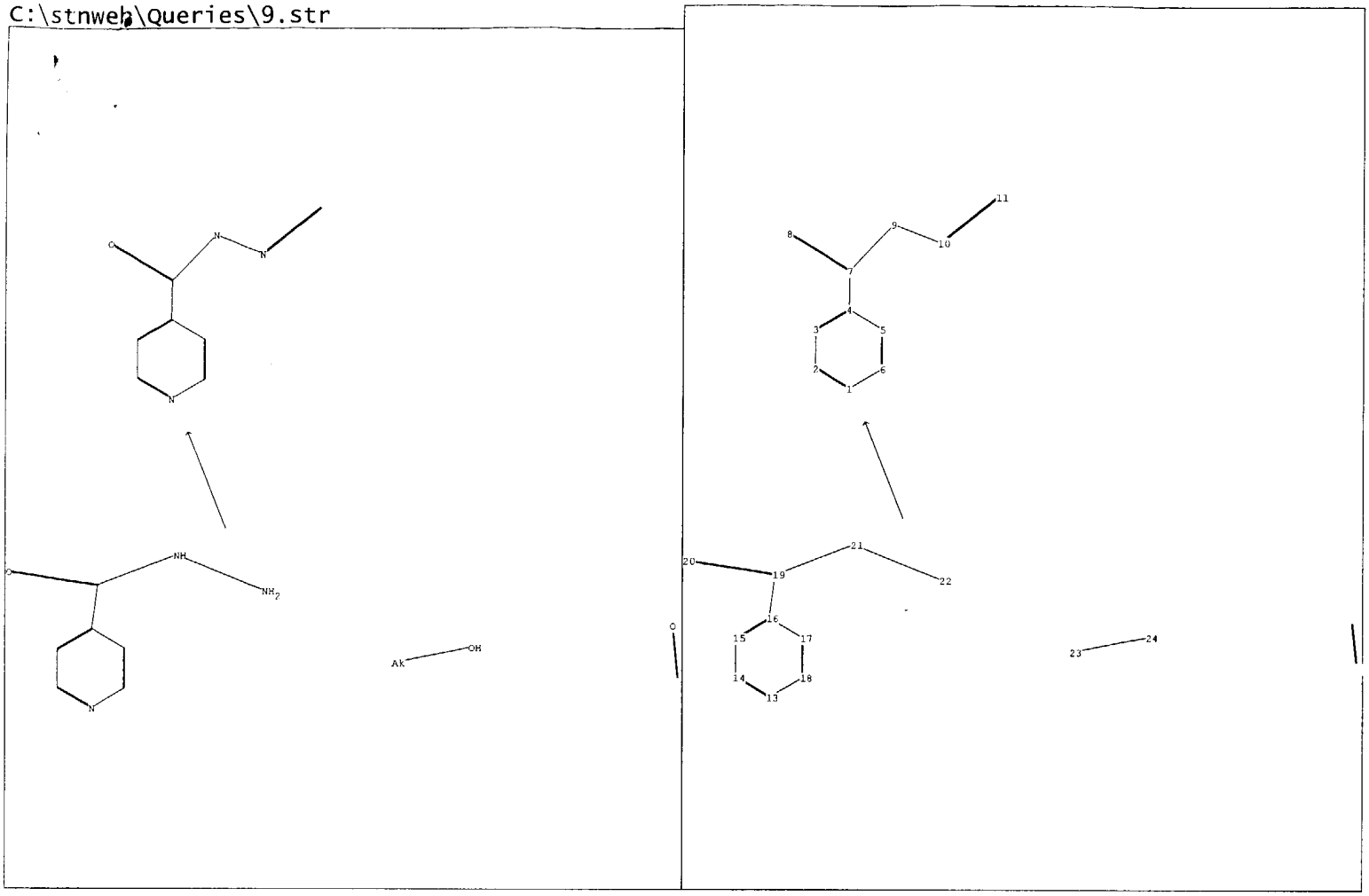
G1:O,S

G2:CH3,Et

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:CLASS 24:CLASS 25:CLASS 28:CLASS 30:CLASS
fragments assigned reactant role:
containing 13
containing 24
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:

containing 28

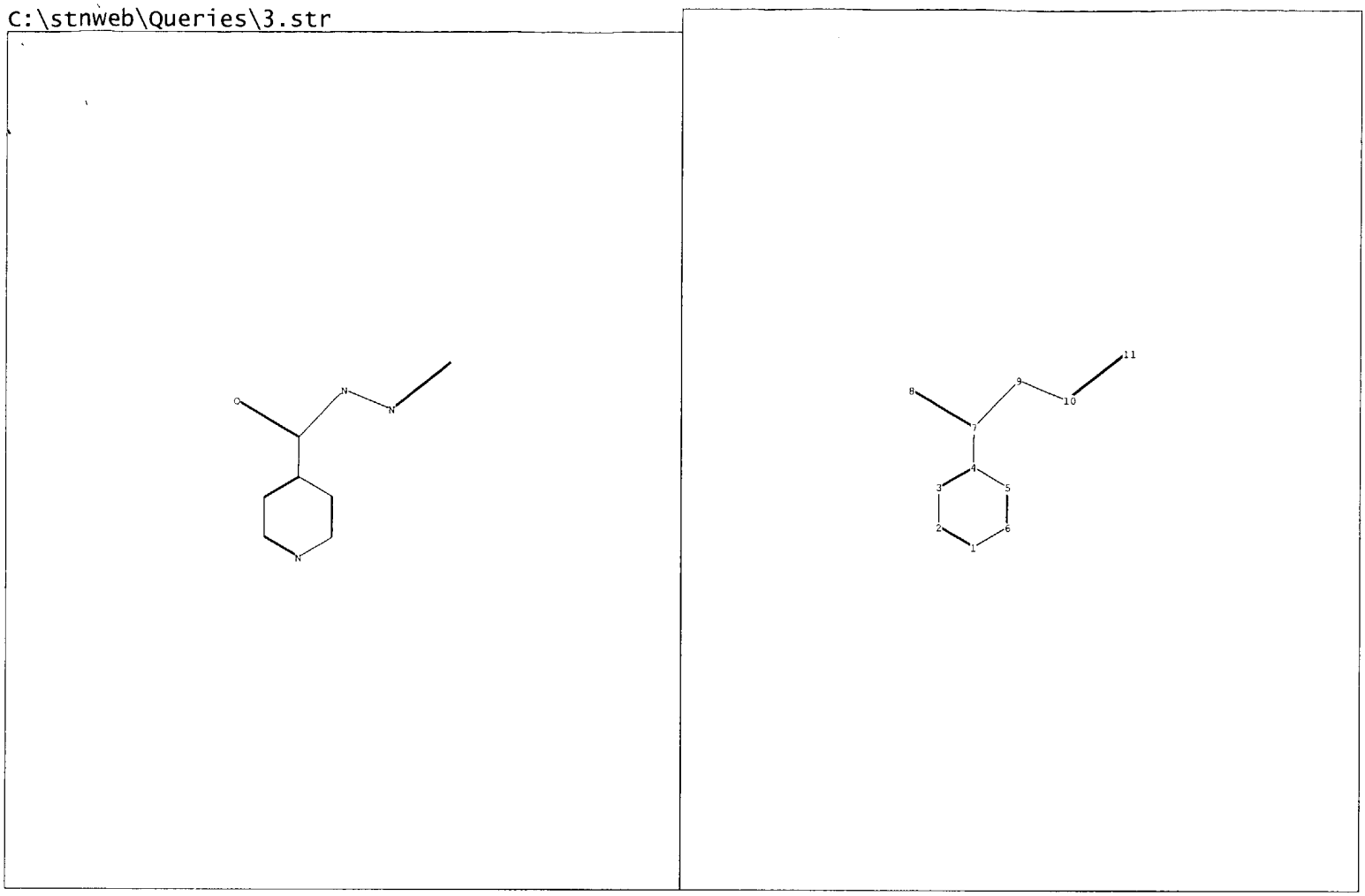
C:\stnweb\Queries\9.str



chain nodes :
7 8 9 10 19 20 21 22 23 24 26
ring nodes :
1 2 3 4 5 6 13 14 15 16 17 18
ring/chain nodes :
11 25
chain bonds :
4-7 7-8 7-9 9-10 10-11 16-19 19-20 19-21 21-22 23-24 25-26
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
exact/norm bonds :
7-8 7-9 9-10 10-11 19-20 19-21 23-24 25-26
exact bonds :
4-7 16-19 21-22
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18
isolated ring systems :
containing 1 : 13 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS 20:CLASS
21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS
fragments assigned reactant role:
containing 13
fragments assigned product role:
containing 1
fragments assigned reactant/reagent role:
containing 23
containing 25

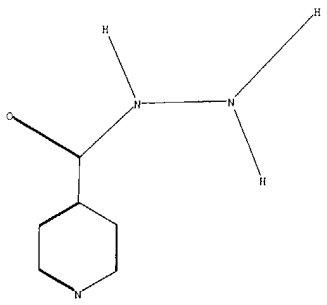
C:\stnweb\Queries\3.str

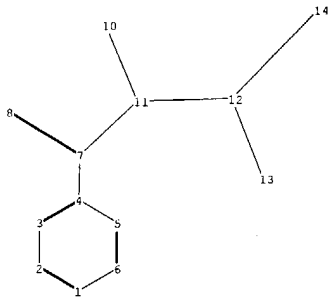


chain nodes :
7 8 9 10
ring nodes :
1 2 3 4 5 6
ring/chain nodes :
11
chain bonds :
4-7 7-8 7-9 9-10 10-11
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
7-8 7-9 9-10 10-11
exact bonds :
4-7
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS
fragments assigned product role:
containing 1

C:\stnweb\Queries\35.str





chain nodes :
7 8 10 11 12 13 14
ring nodes :
1 2 3 4 5 6
chain bonds :
4-7 7-8 7-11 10-11 11-12 12-13 12-14
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
7-8 7-11 11-12
exact bonds :
4-7 10-11 12-13 12-14
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS
fragments assigned product role:
containing 1